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OPserver: interactive online computations of opacities and radiative accelerations

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ABSTRACT

Codes to compute mean opacities and radiative accelerations for arbitrary chemical mixtures using the Opacity Project recently revised data have been restructured in a client–server architecture and transcribed as a subroutine library. This implementation increases efficiency in stellar modelling where element stratification due to diffusion processes is depth dependent, and thus requires repeated fast opacity re-estimates. Three user modes are provided to fit different computing environments, namely, a web browser, a local workstation and a distributed grid.

Key words: atomic processes – radiative transfer – stars: interior.

1 INTRODUCTION

Astrophysical opacities from the Opacity Project (OP) have been updated by Badnell et al. (2005) to include inner shell contributions and an improved frequency mesh. The complete data set of monochromatic opacities and a suite of codes to compute mean opacities and radiative accelerations (RAs) (OPCD_2.1[1]) have also been publicly released by Seaton (2005) to make in-house calculations for arbitrary mixtures more versatile and expedient. Regarding data accuracy, there is excellent overall agreement between the OPAL (Iglesias & Rogers 1996) and OP results as discussed by Seaton & Badnell (2004), Badnell et al. (2005) and Delahaye & Pinsonneault (2005).

Rosseland mean opacities (RMOs) are sensitive to both the basic atomic data used and the assumed abundances of the chemical elements. What had been a good agreement between theory and the helioseismological data was found to be less good using revised solar abundances from Asplund, Grevesse & Sauval (2005). The updated OP opacities have been instrumental in discussions of that problem (Antia & Basu 2005; Bahcall & Serenelli 2005; Bahcall et al. 2005a; Bahcall, Basu & Serenelli 2005b; Bahcall, Serenelli & Basu 2005c; Delahaye & Pinsonneault 2006).

The modelling of stellar interiors, on the other hand, is being renewed with the solar experience. Present (*WIRE*, *MOST*, *CoRoT*) and future (*Kepler*) space probes and the well-established solar methods are giving the field of asteroseismology remarkable growth and the guarantee of invaluable data (Metcalfe, Brown & Christensen-Dalsgaard 2004; Kurtz 2005; Christensen-Dalsgaard 2006). In future work on stellar models it may be desirable to take account of revisions in abundances similar to those performed for the Sun.

For some types of stars, models must take into account microscopic diffusion processes, for example, radiative levitation, gravitational settling and thermal diffusion, as they can affect the internal and thermal structures, the depth of the convection zone, pulsations and give rise to surface abundance anomalies (Seaton 1999; Delahaye & Pinsonneault 2005; Bourge & Alecian 2006). As reviewed by Michaud (2004), such processes are relevant in the

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[1] http://cdsweb.u-strasbg.fr/topbase/op.html

description of chemically peculiar stars, horizontal-branch stars, white dwarfs and neutron stars, and in globular cluster age determinations from Population II turn-off stars. Furthermore, in order to solve the outstanding discrepancy of the atmospheric Li abundance in old stars with that predicted in big bang nucleosynthesis, Richard, Michaud & Richer (2005) have proposed Li sinking deep into the star due to diffusion. This hypothesis has been recently confirmed in the observations by Korn et al. (2006).

The OPCD_2.1 release includes data and codes to compute the radiative accelerations required for studies of diffusion processes. It should be noted that the RAs are summed over ionization stages and that data for the calculation of diffusion coefficients are calculated assuming that the distribution over ionization stages of the diffusing ions is the same as that in the ambient plasma. The validity of this approximation is discussed by Gonzalez et al. (1995).

In some cases, particularly when element stratification depends on stellar depth, calculations of mean opacities and radiative accelerations must be repeated at each depth point of the model and at each time-step of the evolution, and thus the use of codes more efficient than those in OPCD_2.1 may be necessary. This becomes critical in the new distributed computing grid environments where the network transfer of large volumes of data is a key issue. In the present work we have looked into these problems, and, as a solution, report on the implementation of a general-purpose, interactive server for astrophysical opacities referred to as OPserver. It has been installed at the Ohio Supercomputer Center, Columbus, OH, USA, from where it can be accessed through a web page[2] or a linkable subroutine library. It can also be downloaded locally to be run on a stand-alone basis but it will demand greater computational facilities. In Section 2 we discuss the computational strategy of the codes in OPCD_2.1 followed by a description of OPserver in Section 3. In Section 4 we include some tests as an indication of its performance with a final summary in Section 5.

2 OPCD CODES

We highlight here some of the key features of the codes in OPCD_2.1. For a chemical mixture specified by abundance fractions f_k, they essentially compute two types of data: RMOs and RAs.

2.1 Rosseland mean opacities

For the frequency variable

$$u = \frac{h\nu}{k_{\rm B}T}, \tag{1}$$

where $k_{\rm B}$ is the Boltzmann constant, RMOs are given by the harmonic mean of the opacity cross-section $\sigma(u)$ of the mixture:

$$\frac{1}{\kappa_{\rm R}} = \mu \int_0^{v_\infty} \frac{1}{\sigma(u)}\,{\rm d}v, \tag{2}$$

where μ is the mean atomic weight. The $\sigma(u)$ is a weighted sum of the monochromatic opacity cross-sections for each of the chemical constituents:

$$\sigma(u) = \sum_k f_k \sigma_k(u), \tag{3}$$

and is conveniently tabulated on the v mesh:

$$v(u) = \int_0^u \frac{F(u)}{1-\exp(-u)}\,{\rm d}u, \tag{4}$$

[2] http://opacities.osc.edu

where

$$F(u) = \frac{15u^4\exp(-u)}{4\pi^4[1-\exp(-u)]^2} \tag{5}$$

and $v_\infty = v(u \rightarrow \infty)$. The rationale behind the v mesh is that it enhances frequency resolution where $F(u)$ is large (Badnell et al. 2005).

2.2 Radiative accelerations

Similarly, the RAs for a selected k element can be expressed as

$$g_{\rm rad} = \frac{\mu\kappa_{\rm R}\gamma_k}{c\mu_k}\mathcal{F}, \tag{6}$$

where μ_k is its atomic weight and c the speed of light. The function $\mathcal{F}$ is given in terms of the effective temperature $T_{\rm eff}$ and fractional depth $r/R_\star$ of the star by

$$\mathcal{F} = \pi B(T_{\rm eff})\left(\frac{R_\star}{r}\right)^2 \tag{7}$$

with

$$B(T) = \frac{2(\pi k_{\rm B}T)^4}{15c^2h^3}. \tag{8}$$

The dimensionless parameter

$$\gamma_k = \int \frac{\sigma_k^{\rm mta}}{\sigma}\,{\rm d}v \tag{9}$$

depends on the cross-section for momentum transfer to the k element

$$\sigma_k^{\rm mta} = \sigma_k(u)[1-\exp(-u)] - a_k(u), \tag{10}$$

where $a_k(u)$ is a correction to remove the contributions of electron scattering and momentum transfer to the electrons. Both $\sigma_k(u)$ and $a_k(u)$, which are hereafter referred to as the MONO data set (∼1 GB), are tabulated in equally spaced v intervals to facilitate accurate interpolation schemes.

2.3 Computational strategy

The computational strategy adopted in the OPCD_2.1 release is depicted in the flowcharts of Fig. 1 where it may be seen that calculations of RMOs and RAs are carried in two stages. In a time-consuming Stage 1, RMOs and RAs are computed with the MIXV and ACCV codes, respectively, on a representative tabulation of the complete temperature–electron density (T, $N_{\rm e}$) plane. In MIXV the chemical mixture is specified in the input file mixv.in as

$$\{X, Z, N, Z_k, f_k\}, \tag{11}$$

where X and Z are the hydrogen and metal mass fractions, N the number of elements and Z_k and f_k are the metal nuclear charges and fractional abundances. In ACCV, the input data (accv.in) are

$$\{N, Z_k, f_k, Z_i, N_\chi, \chi_j\}, \tag{12}$$

where now k runs over the N elements of the mixture, and Z_i and χ_j are, respectively, the nuclear charge and N_χ abundance multipliers of the test i element. Input data formats in either mixv.in or accv.in give the user flexible control over chemical mixture specifications.

As shown in Fig. 1, the intermediate output files mixv.xx (∼85 kB) containing

$$\{\rho, \kappa_{\rm R}\}(T, N_{\rm e}), \tag{13}$$

where ρ is the mass density, and acc.xx (∼470 kB) with

$$\left\{\kappa_{\rm R}, \frac{\partial\kappa_{\rm R}}{\partial\chi}, \gamma, \frac{\partial\gamma}{\partial\chi}\right\}(T, N_{\rm e}, \chi_j) \tag{14}$$

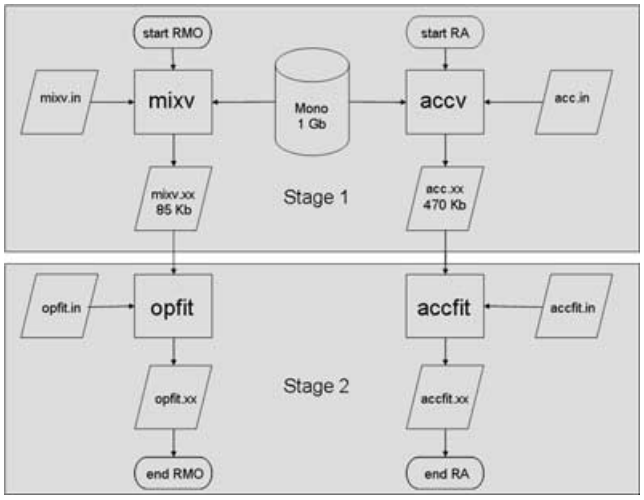

Figure 1. Flowcharts for the computations of RMOs and RAs with the codes in the OPCD_2.1 release. They are carried out in two stages: in a time-consuming Stage 1, data are computed for the whole (T, N_e) plane followed by fast bicubic interpolations in Stage 2. The intermediate files mixv.xx and acc.xx enable communication between these two steps.

are written to disc. They are then, respectively, read by the codes OPFIT and ACCFIT in Stage 2 for fast bicubic interpolations of RMOs and RAs on stellar depth profiles $\{T, \rho, r/R_\star\}$ (i) specified by the user in the opfit.in and accfit.in input files. The final output files are opfit.xx containing

$$\left\{\log\kappa_{\rm R}, \frac{\partial\log\kappa_{\rm R}}{\partial\log T}, \frac{\partial\log\kappa_{\rm R}}{\partial\log\rho}\right\}(i) \tag{15}$$

and accfit.xx with

$$\{\log\kappa_{\rm R}, \log\gamma, \log g_{\rm rad}\}(i, \chi_j). \tag{16}$$

In this computational approach, performance is mainly limited by the summation in equation (3) which implies disc reading the MONO data set; for instance, in MIXV it takes up to ∼90 per cent of the total elapsed time. OPCD_2.1 also includes other codes such as MX and AX which, respectively, compute RMOs and RAs for a star depth profile. The chemical mixture can be fully varied at each depth point using the specifications in equations (11) and (12), the RMOs and RAs being obtained in a one-step process using bicubic interpolations without splines. These methods are thus suitable for cases with multimixture depth profiles (Seaton 2005). Further details of all the OPCD codes are contained in the reference manual.[3]

3 OPSERVER

In OPserver the computational capabilities of the codes in OPCD_2.1 are greatly enhanced by the following innovative adaptations.

(i) The codes are restructured within a client–server network architecture whereby the time-consuming Stage 1 is performed on a powerful processor while the fast Stage 2 is moved to the client, for example, a web server or a user workstation. In this arrangement performance could be affected by the client–server transfer of the mixv.xx and acc.xx intermediate files, but since they are never larger than 0.5 MB, it is not expected to be a deterrent with present-day bandwidths. In a local installation where both the client and server reside on the same machine, communication is managed through shared buffers in main memory; that is, the corresponding data in mixv.xx and acc.xx are not written to disc.

(ii) The codes are transcribed as a subroutine library – to be referred to hereafter as the OPlibrary – which can be linked by the user stellar modelling code for recurrent subroutine calls that avoid data writing on disc. That is, the input data in the mixv.in, accv.in, opfit.in and accfit.in files and the output tables in the opfit.xx and accfit.xx files (see Fig. 1) are now handled as subroutine parameters while the intermediate mixv.xx and acc.xx files are passed via shared main-memory buffers. Chemical mixtures are again specified with the formats of equations (11) and (12) which allow full variation at each depth point in a single subroutine call.

(iii) RMOs/RAs are computed with the complete MONO data set always loaded in main memory thus avoiding lengthy and repeated disc readings. This is achieved by implementing OPserver on a dedicated server where MONO is permanently resided in RAM, or in the case of a local installation, by disc reading once at the outset of a modelling calculation.

(iv) When accessing the remote server, client data requests are addressed through the HTTP protocol, that is, in terms of a Uniform Resource Locator (URL). This allows data fetching from the central facility through an interactive web page or a network access subroutine, the latter being particularly suitable for a stellar model code that is to be run in a distributed grid environment.

(v) The DO-LOOP that computes the summation of equation (3) has been parallelized in OpenMP which provides a simple, scalable and portable scheme for shared-memory platforms.

As shown in Fig. 2, the current OPserver enterprise is implemented as a client–server model at the Ohio Supercomputer Center (OSC). The web server communicates with the supercomputer via a socket interface. Earlier versions were developed on an SGI Origin2000 server with the PowerFortran parallelizing compiler. The current version runs on a Linux system with Fortran OpenMP directives. OPserver offers three user modes with full

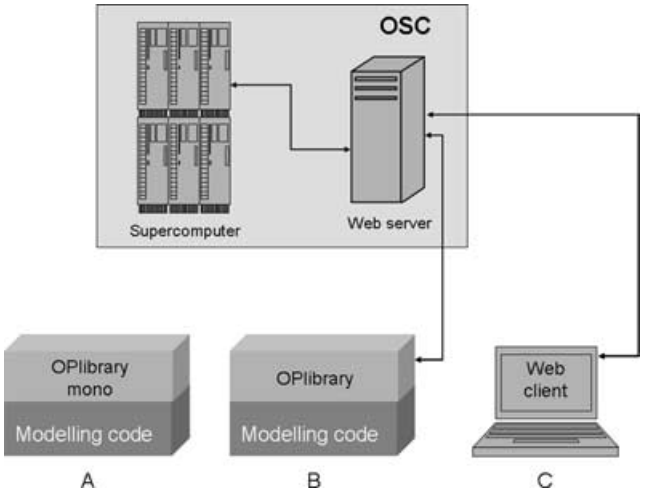

Figure 2. OPserver enterprise showing the web server–supercomputer tandem at the OSC and the three available user modes. (a) The OPlibrary and monochromatic opacities (MONO) are downloaded locally and linked to the user modelling code such that RMOs/RAs are computed locally. (b) The OPlibrary is downloaded locally and linked to the modelling code but RMOs/RAs are computed remotely at the OSC. (c) RMO/RA computations at the OSC through a web client.

[3] http://opacities.osc.edu/publi/OPCD.pdf

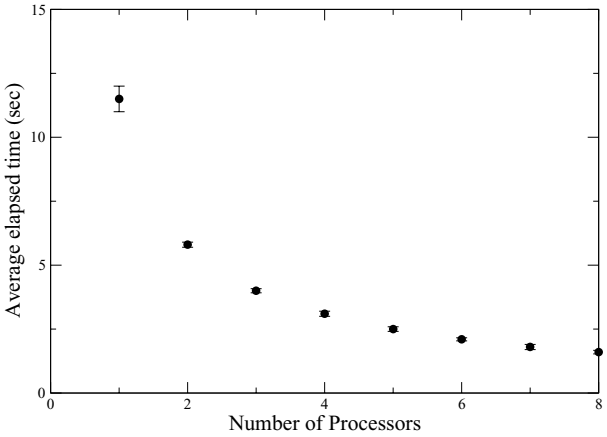

Figure 3. Average elapsed time for the computation of RMOs (Stage 1) in OPserver as a function of the number of processors on an SGI Origin2000 showing the acceleration obtained through parallelism. The corresponding time taken by the MIXV code for this calculation is 140 s where the time taken by data reading from disc is 126 s.

functionality except when otherwise indicated in the following description.

Mode A: In this mode OPserver is set up locally on a stand-alone basis (see Fig. 2). The facilities of the OSC are not used. A new OPCD release (OPCD_3.3[4]) is downloaded, followed by (i) installation of both the OPlibrary and the MONO data set and (ii) linking of the OPlibrary to the user modelling code. Computations of RMOs/RAs are preceded by the reading of the complete MONO data set from disc and therefore requires at least 1 GB of RAM.

Mode B: In this mode, the OPlibrary is downloaded, installed and linked to the user code, but Stage 1 is performed remotely at the OSC (see Fig. 2). This option has been customized for stellar modelling in a distributed grid environment that would otherwise imply (i.e. Mode A) the network transfer, installation and disc reading of the MONO data set at runtime. It is also practical when local computer capabilities (RAM and/or disc space) are limited. The functions provided by the MX and AX codes have not been implemented.

Mode C: In this mode RMO/RA computations at the OSC are requested through an interactive web page[5] which allows both Stages 1 and 2 to be carried out remotely or, alternatively, Stage 2 locally by downloading the mixv.xx/acc.xx intermediate files (see Fig. 1) with the browser for further processing with local OPFIT/ACCFIT executables.

4 TESTS

OPserver benchmarks were initially carried out on an SGI Origin2000 multiprocessor at the OSC with an earlier release of OPCD. For the standard S92 mixture (Seaton et al. 1994), the MIXV code took up to 140 s to compute the mixv.xx file, of which 126 s were dedicated to disc reading and 14 s to the actual computing of the mean opacities. OPserver took on average 12.0 ± 0.5 s to compute mixv.xx which was not written to disc unless requested. In Fig. 3 we show the acceleration obtained on the Origin2000 through parallelization where the calculation of mean opacities is reduced to 2 s with eight processors. Further significant acceleration is prevented by data transfer overheads.

On more recent workstations, the local performances of the codes in OPCD_2.1 and OPserver depend on processor speed and RAM and cache sizes. For instance, on a PowerMac G5 (PowerPC 970fx processor at 2.0 GHz, 1 GB of RAM and L2 cache of 512 kB) the first time MIXV is run it takes for a single S92 mixture 103.8 s to compute the RMOs, but on subsequent runs the elapsed time is reduced to an average of 28.2 ± 0.2 s. Similarly, OPserver takes 103.3 s which is then reduced to 31.4 ± 0.4 s on subsequent runs. Once the MONO data set is loaded in RAM by OPserver (Mode A), calculations of RMOs for a single S92 mixture only take 5.29 ± 0.02 and 6.13 ± 0.01 s for RAs for the test element Ar. In Mode B, where Stage 1 is carried out remotely at the OSC and the mixv.xx and accv.xx files are transferred at the relatively low rate of 1.88 kB s^{-1}, computations of RMOs and RAs take 5.9 ± 0.1 and 9.3 ± 0.3 s, respectively. The noticeable longer time taken for the latter is due to the transfer time taken for the larger accv.xx file.

5 SUMMARY

RMOs and RAs can be computed from OP data in any one of the following ways.

(i) Download the original OPCD_2.1 package as described by Seaton (2005) and perform all calculations locally.

(ii) Mode A, download the upgraded OPCD_3.3 package, install OPserver and perform all calculations locally by linking the subroutines in the OPlibrary. Calculations with OPserver are more efficient but require large local computer memory.

(iii) Mode B, as Mode A but with Stage 1 performed remotely at the OSC. Mode B is convenient if fast calculations are required but local computer memory is limited or when stellar modelling is to be carried out in a grid environment.

(iv) Mode C, perform all calculations remotely at the OSC through an interactive web page whereby files are downloaded locally with the browser.

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